Increasing the Coverage of Medicinal Chemistry-Relevant Space in Commercial Fragments Screening

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Table S1 Frequent bioactive ChEMBL substructures that have

low similarity to commercial fragments S2

Table S1. The most frequently occurring substructures derived from a minimum of 100 bioactive ChEMBL compounds that have low similarity to commercial fragments. The frequency occurrence of each substructure is denoted below the structure.

N 0	N N	O N	O N
618	466	439	413
0 N		N N N N N N N N N N N N N N N N N N N	
271	246	215	213
205	% - Z 198	888	188 × Z × Z
180	169	N 168	159

